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13. ABSTRACT *(Maximum 200 words)*

We made significant progress in each of these general areas. We produced high resolution models and codes that simulate molten fiber manufacturing processes. We have further completed new inverse models and experiments by colleagues at the Department of Agriculture and Chemical Engineering at Ohio State University, which provide state-of-the-art material characterization of dynamic surface tension, elongational viscosity, and elastic relaxation.

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Final Technical Report

Toward Technological Application of Non-Newtonian Fluids and Complex Materials: Modelling, Simulation, and Design of Experiments

AFOSR Grant/Contract No. F49620-93-~~10525~~ 0431 93-1-0431

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OBJECTIVES

1. Modeling of fiber flows: incorporation of physics important in industrial processes

2. Design of experiments and compatible models for inverse problems and material characterization

RESEARCH RESULTS

We made significant progress in each of these general areas. We produced high resolution models and codes that simulate molten fiber manufacturing processes. We have further completed new inverse models and experiments by colleagues at the Department of Agriculture and Chemical Engineering at Ohio State University, which provide state-of-the-art material characterization of dynamic surface tension, elongational viscosity, and elastic relaxation.

ACCOMPLISHMENTS/NEW FINDINGS

1. We have now successfully modelled and incorporated into online industrial codes (for Hoechst Celanese Corporation):

a. The models and codes compute the radial dependence of temperature and stress within the filament. Transverse variations of these quantities within the filament lead to production problems(breaks) and fiber performance problems
(nonuniform tensile strength). The resolution of transverse temperature and stress variations in filaments during melt spinning is an important tool in reducing these variations, and hence these problems. Previous models for filament manufacturing compute only the axial evolution of the cross-sectional averages of these quantities.

b. Change-of-phase along the spinline is now resolved as a freeze surface that varies transversely as well as axially.

c. Multifilament coupling in spinning processes is now modeled entirely based on first principles, predicting the quite different cooling, airflow, and drag effects experienced by different rows of filaments. The models and codes therefore predict the resulting fiber-to-fiber nonuniformity in a bundle of fibers.

d. The models and codes fundamentally couple internal
orientation to the hydrodynamics and thermodynamics of fiber spinning. This
work
was critical for replacing empirical stress-optical laws used in industry
with a
first-principles prediction of the evolution of stress and birefringence
during
melt spinning.

2. We have made progress in academic settings addressing other issues of
technological
importance:

a. Recovery of the Rayleigh capillary instability results from slender asymptotic models derived from Navier-Stokes equations with a free surface. Extension of these results to fluids with rigid-rod microstructure.

b. We derived the thermomechanical equations governing a material
with prescribed
temperature-dependent density. Thermal shrinkage effects are important
in polymer
processing. Conventional modeling merely inserts a temperature-dependent
density
a posteriori into the equations governing an incompressible material, thereby violating the second law of thermodynamics. When applying our
thermodynamically
consistent model to the test problem of flow through a channel, we not only predicted features completely missed by the conventional treatment, but also uncovered fundamental problems in the underlying theory of thermomechanically constrained materials, which we are now pursuing.

c. We have extended the modeling to multicomponent filaments.

3. Significant progress has been achieved in material characterization:

a. Material characterization of dynamic surface tension and elongational viscosity through inverse models for oscillating jets has been successfully completed. This work has been published with the Department of Agriculture, where they do the experiments and we do the modeling and computation.

b. Sub-millisecond variations in surface tension have been resolved in a new model for surfactant transport in spray applications. This resolution is necessary to accurately predict (and regulate) the dominant lengthscales of drop formation. This facility is also relevant to other industrial applications such as microencapsulation.

c. A new experimental apparatus (by K. Koelling of Chem. Eng. at OSU) together with our viscoelastic modeling has led to characterization of relaxation times and elongational viscosity in fiber spinning flows. This advance is critical to transfer of these effects to online codes.

PERSONNEL SUPPORTED

Faculty: M. Gregory Forest and Stephen E. Bechtel

Post-Docs: None

Graduate Students: C. David Carlson

N.B. My recent student, C.D. Carlson, is currently employed by Hoechst Celanese Corporation.

PUBLICATIONS

``Torsional effects in high-order viscoelastic thin-filament models,'' S. Bechtel, K. Bolinger, M. G. Forest, J. Cao, SIAM J. Appl. Math. 55(1), 1995, pp. 58-99.

``A new model to determine dynamic surface tension and elongational viscosity using oscillating jet measurements'', S. E. Bechtel, J. A. Cooper, N. A. Petersson, D. L. Richard, A. Saleh, V. Ramanan, Journal of Fluid Mechanics 293, 1995, pp. 379-403.

``Modeling and computation of the onset of failure in polymeric liquid filaments'', S. E. Bechtel, M. G. Forest, Q. Wang, Journal of Non-Newtonian Fluid Mechanics 58, 1995, pp. 97-129.

"Recovery of the Rayleigh Capillary Instability from Slender 1-D Inviscid and Viscous Models", S. Bechtel, C.D. Carlson, and M.G. Forest, Physics of Fluids 7 (12), December, 1995, pp. 2956-2971.

"Thermomechanical Equations Governing a Material with Prescribed Temperature-Dependent Density, with Applications to Nonisothermal Plane Poiseuille Flow", D. Cao, S. Bechtel, and M.G. Forest, Journal of Applied Mechanics 63(4), 1996, pp. 1011-1018.

"1-D Models for Thin Filaments of Liquid Crystalline Polymers: Coupling of Orientation and Flow in the Stability of Simple Solutions", M. G. Forest, Q. Wang, and S. Bechtel, Physica D: Nonlinear Phenomena 99(4), 1997, pp. 527-554.

"Exploiting Accurate Spinline Measurements for Material Characterization", V. Ramanan, V. Gauri, K. Koelling, S. Bechtel, and M. G. Forest, Journal of Rheology 41(2), 1997, pp. 1-24.

``One dimensional isothermal spinning models for liquid crystalline polymer fibers'', M. G. Forest, Q. Wang, S. E. Bechtel, Journal of Rheology 41(4), 1997, pp. 821-850.

INTERACTIONS/TRANSITIONS

*Participation/Presentations:

Colloquia at the University of North Carolina at Charlotte (10/26/95), the University of Indiana (1/19/96).

Presentation to the Optical Fiber Manufacturing Seminar of Corning, INC., Wilmington, NC (4/2/96).

Presentations to the Technical Fibers Group of Hoechst Celanese Corporation, Charlotte, NC (4/8/95, 10/18/96, 7/17/97).

Invited presentations at Conferences: Penn State University Applied Mathematics Workshop for Materials Studies and Industrial Applications, 10/18/96; Hoechst Celanese Corporation/ University of North Carolina Polymer Workshop, 11/7/96; IVth Workshop on PDEs, IMPA, Brazil, 7/18/95; Society of Rheology Annual Meeting, Galveston, TX, 2/16/97; 17th Annual Conference of the Center for Nonlinear Studies, Los Alamos National Laboratory, 5/16/97; Siam Meeting in Philadelphia, PA, 5/12/97.

*Consultative Functions:

Forest and Bechtel currently develop and maintain and upgrade the fiber spinning model and code for Hoechst Celanese Corporation, Charlotte, NC.

Further, we have visited and discussed with Corning, INC. issues related to the manufacture of optical fibers.

*Transitions:

Our new generation code, Multfil3, for Hoechst Celanese Corporation, which computes the radial dependence of stress and temperature in the filament, has been effectively used to help remove transverse variations in fibers. The next generation code, Multfil4, which in addition computes the fundamentally coupled evolution of birefringence along the filament, has just been delivered. This transition can be verified by Kenneth Giese, 704-554-3276. As always, we can provide written non-disclosing statements from HCC to this effect.

NEW DISCOVERIES

None.

HONORS/AWARDS

None.